Complex coupled-cluster approach to an *ab-initio* description of open quantum systems

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We develop *ab-initio* coupled-cluster theory to describe resonant and weakly bound states along the neutron drip line. We compute the ground states of the helium chain $^{3-10}$He within coupled-cluster theory in singles and doubles (CCSD) approximation. We employ a spherical Gamow-Hartree-Fock basis generated from the low-momentum N^{3}LO nucleon-nucleon interaction. This basis treats bound, resonant, and continuum states on equal footing, and is therefore optimal for the description of properties of drip line nuclei where continuum features play an essential role. Within this formalism, we present an *ab-initio* calculation of energies and decay widths of unstable nuclei starting from realistic interactions.

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Exotic phenomena emerge in weakly bound and resonant many-body quantum systems. These phenomena include ground states that are embedded in the continuum, melting and reorganizing of shell structures, extreme matter clusterizations and halo densities. These unusual features occur in many branches of physics; as examples, we mention Fano resonances [1] in quantum dots [2], ultracold atom gases [3], auto-ionizing atoms [4] or molecules [5], and exotic nuclei. In nuclear physics we find such exotic systems moving away from the valley of nuclear stability towards the drip lines, where the outermost nucleons literally start to drip from the nuclei.

The theoretical description of weakly bound and unbound quantum many-body systems is a challenging undertaking. The proximity of the scattering continuum in these systems implies that they should be treated as open quantum systems where coupling with the scattering continuum can take place. Recent work with Gamow states employed in Hamiltonian diagonalization methods [6, 7, 8, 9, 10] have shown that these basis states correctly depict properties associated with open quantum systems. This Berggren basis is composed of bound, resonant, and (continuum) scattering single-particle states [11]. This basis significantly improves and facilitates the description of loosely bound systems and is essential in the description of unbound systems. However, the typically large number of discretized continuum states limits this approach to traditional shell-model diagonalization calculations where an inert core is employed.

In this Letter, we present an *ab-initio* approach to open quantum systems using a Gamow-Hartree-Fock basis derived from realistic interactions [8]. We employ coupled-cluster theory [12, 13, 14, 15, 16, 17, 18, 19, 20] to solve the quantum many-body problem for the helium chain in this basis. Coupled-cluster techniques computationally scale much more gently with increasing system size, than exact diagonalization methods, and are therefore very well suited for open quantum systems where the number of orbitals are typically orders of magnitude larger than for closed quantum systems. Its application with Gamow basis states is based on a non-Hermitian representation of the many-body Hamiltonian. This is a rather new direction in coupled-cluster theory [21], and we report its first successful application in nuclear theory. Other *ab-initio* methods like the Green's function Monte Carlo [22] or the no-core shell model [23] have previously been employed to compute the structure of helium isotopes.

This Letter is organized as follows. We first introduce coupled-cluster theory, the interaction and the model space. Second, we provide several checks to gauge the accuracy of our approach by comparison with exact diagonalization methods. Third, we perform large-scale calculations of the ground states of helium isotopes.

Method and model space. In coupled-cluster theory we make the exponential ansatz for the exact correlated ground state,

$$|\Psi\rangle = \exp(T)|\Phi_0\rangle \ . \tag{1}$$

Here $|\Phi_0\rangle$ is an uncorrelated reference Slater determinant which might be either the Hartree-Fock (HF) state or a naive filling of the oscillator single-particle basis. Correlations are introduced through the exponential $\exp(T)$ operating on $|\Phi_0\rangle$. The operator T is a sum of n-particle–n-hole excitation operators $T = T_1 + T_2 + ...$ of the form,

$$T_n = \sum_{a_1 \ldots a_n, i_1 \ldots i_n} t_{i_1 \ldots i_n}^{a_1 \ldots a_n} a_{a_1}^\dagger \cdots a_{a_n}^\dagger a_{i_n} \cdots a_{i_1} \ , \tag{2}$$

where $i_1, i_2, ...$ are summed over hole states and $a_1, a_2, ...$ are summed over particle states. One obtains the algebraic equation for the excitation amplitudes $t_{ij\ldots}^{ab\cdots}$ by left-projecting the similarity-transformed Hamiltonian with an n-particle–n-hole excited Slater determinant giving

$$\langle \Phi_{ij\ldots}^{ab\cdots}| \left(H_N \exp(T)\right)_C |\Phi_0\rangle = 0 \ , \tag{3}$$

where the Hamiltonian enters in normal-ordered form, and the subscript C indicates that only connected diagrams enter. We iteratively solve the non-linear set of coupled equations (3) for the excitation amplitudes. The solutions determine the coupled-cluster correlation energy

$$E_{\rm CC} = \langle\Phi_0| \left(H_N \exp(T)\right)_C |\Phi_0\rangle \ . \tag{4}$$

In this work, we truncate the cluster operator T at the two-particle–two-hole level (CCSD), i.e. we approximate $T = T_1 + T_2$. We also investigate whether the perturbative triples correction CCSD(T) [24] improve on the CCSD results.

We construct our basis using the Berggren formalism [11] in which bound, resonant and continuum states are treated on equal footing. The Berggren basis is an analytic continuation of the usual completeness relation in the complex energy plane. The representation of the Hamiltonian in a finite Berggren basis is no longer Hermitian but rather complex symmetric, and renders the coupled-cluster equations (3) and (4) complex.

The nuclear Hamiltonian is given by

$$H = t - t_{\rm CoM} + V \ . \tag{5}$$

Here, t denotes the operator of the kinetic energy, and $t_{\rm CoM}$ is the kinetic energy of the center of mass. The nucleon-nucleon interaction V is based on chiral effective field theory within the N^{3}LO expansion [25]. This potential is a systematic momentum-space expansion to fourth order of a Lagrangian that obeys QCD symmetries. It contains high-momentum components and is therefore not suitable for the limited basis sets we employ. In order to make the calculation feasible, we construct a low-momentum interaction $V = V_{{\rm low}-k}$ following the formalism outlined in [26]. This is done by integrating out those high-momentum modes of the chiral potential that exceed the chosen momentum cutoff Λ. The construction of $V_{{\rm low}-k}$ is a renormalization group transformation and therefore generates three-body forces and also forces of higher rank. These forces depend on the cutoff, and only the sum of all forces is cutoff-independent. In this work, we limit ourselves to two-body forces. Since we are interested in helium isotopes, $\Lambda = 1.9{\rm fm}^{-1}$ is a *convenient* choice, as the ground state expectation value of the omitted three-nucleon force is very small for ^{3}H and ^{4}He [27].

We build our coupled-cluster reference state from a single-particle basis obtained through a self-consistent Gamow-HF calculation [8]. For the helium isotopes considered in this work, the proton separation energy is typically of the order of $20-30$ MeV, and protons mainly occupy deeply bound s-orbits. The situation is different for the neutrons where in neutron-rich systems the separation energy is very small. Furthermore, neutrons in p-orbits are believed to build up the main part of surface densities. Based on these observations we use harmonic oscillator wave functions (with $\hbar\omega = 20$ MeV) for the protons and for the higher partial waves ($d-g$ waves) on the neutron side. For neutrons in s and p orbits, we use a complex Woods-Saxon basis where the non-resonant continuum is defined on a triangular contour in the complex k-plane (see Fig. 3 in Ref. [8] for details). Using Gauss-Legendre quadrature, the discretization of L^+ has been carried out with 3 points in the interval $(0, A)$, 4 points in the interval (A, B), and 13 points in the interval (B, C). Consequently, for each of the s-p partial waves on the neutron side, we have a discretized basis built from bound, resonant, and non-resonant continuum states. For all other partial waves on the proton and neutron side, we use an oscillator basis with the energy truncation $N = 2n + l \leq 10$. This combination of complex Woods-Saxon states for low values of angular momentum and harmonic oscillator states for higher values of angular momentum captures the relevant physics and keeps the total size of the single-particle basis manageable. We find good convergence of the HF energy with respect to the number of integration points and size of our single-particle model space.

Accuracy of the Coupled-Cluster method. Weakly bound and resonant nuclei present a double challenge to the coupled-cluster method. First, some of the considered helium isotopes have open-shell character. Such systems are more difficult to describe within single-reference coupled-cluster methods. Second, particle-unstable nuclei like ^{5,7}He have resonant ground states. Here, the physical ground state is not the ground state of the model space we employ since scattering states might have lower energies. We develop a procedure which allows one to identify the physical state on the many-particle energy surface. Both problems are addressed in what follows.

To study the accuracy for open-shell nuclei, we compare the CCSD energies of $^{3-6}$He with exact results obtained through diagonalization. We restrict ourselves to Hamiltonians represented in a finite oscillator space, and thereby separate open-shell aspects from properties related to open systems. The exact diagonalization is only possible in a relatively small model space consisting of s, p, and d states up to the $4s3p1d$ oscillator states. The results are presented in Table I. The CCSD calculations use a reference Slater determinant built from a spherical oscillator (OSC) basis, from a spherical spin-restricted HF basis (RHF), and from a semi-canonical HF basis in which the Fock-matrix is diagonal in the hole/hole and particle/particle subspaces (SC-RHF). The basis sets are spherically symmetric, and there is a freedom in defining a reference Slater determinant for open-shell nuclei. For a nucleus with known spin J, we define our reference state such that its total spin projection is maximal. Furthermore, the orbits with largest absolute value of the spin projection m_j are filled first. For example, for ^{6}He we place the two outermost neutrons in the

$m_j = 3/2, -3/2$ orbitals for the ground state calculation. In Table I we compare the results from diagonalization with the CCSD results and with triples-corrected results (CCSD(T)). The perturbative triples corrections are calculated using converged T_1 and T_2 amplitudes. For $^{3-5}$He the CCSD results differ by not more than 500 keV from the exact results. Triples corrections improve this deviation to 200 keV (or less). For the open-shell nucleus ^{6}He, the CCSD results differ by 1.7 MeV from the exact result, including triples correction the error decreases to 200 keV.

Method	^{3}He	^{4}He	^{5}He	^{6}He
CCSD (OSC)	-6.21	-26.19	-21.53	-20.96
CCSD (RHF)	-6.10	-26.06	-21.55	-20.99
CCSD (SC-RHF)	-6.11	-26.06	-21.55	-21.04
CCSD(T) (OSC)	-6.40	-26.30	-21.91	-22.83
CCSD(T) (RHF)	-6.35	-26.24	-21.90	-22.56
CCSD(T) (SC-RHF)	-6.34	-26.24	-21.91	-22.62
Exact	-6.45	-26.3	-22.1	-22.7

TABLE I: Comparison of CCSD results and triples-corrected CCSD(T) results with exact calculations for the ground states of helium isotopes. The energies E are given in MeV, and the results are displayed for different basis sets as described in the text.

Using different basis sets, the CCSD(T) results for $^{3-5}$He do not vary by more than $\sim$ 60keV, indicating improved convergence with CCSD(T). However, for ^{6}He the CCSD(T) results vary by $\sim$ 300keV for the different basis sets used. This indicates that the perturbative triples correction CCSD(T) is not tenuous for the nucleus ^{6}He, and that the triples clusters have to be treated more accurately for truly open-shell nuclei [28, 29].

To study the accuracy of CCSD for particle-unstable nuclei, we consider the problem of ^{7}He (using a ^{4}He core) and compare with exact diagonalizations. Recall that the resonant state is embedded in a (quasi) continuum of scattering states. Thus, one must construct a procedure to identify it. Within CCSD, we use a reference state built from bound and resonant single-particle orbitals. Therefore, the reference state is a localized state in the Gamow-HF basis and the CCSD correlations are built upon it. Our model space for ^{7}He consists of nine $p_{3/2}$ orbitals above the ^{4}He core. The exact diagonalization yields a resonant state at energy $E = 2.37$MeV and width $\Gamma = 0.23$MeV, our CCSD result deviates from this result by less than 10 keV. We also checked that the results reported in this Letter show good convergence with respect to the number of discretization points of the contour L^+, and with respect to changes of the oscillator frequency of the basis states we employ. We estimate the error due to the limited discretization, to be within 100 keV for the real part and 20keV for the imaginary part of the energy.

Results. We now turn to large-scale CCSD calculations for $^{3-10}$He isotopes. Table II presents the converged CCSD ground state energies for the $^{3-10}$He isotopes for increasing number of partial waves in our single-particle basis. Here, *s-p* refers to a $5s5p$ proton and $20s20p$ neutron space; *s-d* refers to a $5s5p5d$ proton and $20s20p5d$ neutron space; *s-f* refers to a $5s5p5d4f$ proton and $20s20p5d4f$ neutron space; finally *s-g* refers to a $5s5p5d4f4g$ proton space and a $20s20p5d4f4g$ neutron space, respectively. For our *s-g* calculation we have a total of 556 single-particle states. The computed widths and lifetimes of the helium isotopes are in semi-quantitative agreement with experiment. Our CCSD calculations correctly depict that ^{5}He and ^{7}He are unbound while ^{8}He is bound in their ground states. At the CCSD level, ^{6}He is nearly bound in its ground state. We found that the perturbative triples correction (T) to the ground state of ^{6}He does not improve on the CCSD results. We also found that the triples correction differs considerably using approximate or fully converged T_1 and T_2 amplitudes. This is contrary to what is typically found in quantum chemistry, and suggests that a perturbative treatment becomes invalid. It might be that the HF state is not a good starting point for a perturbative expansion and/or that the high density of continuum states makes perturbation theory break down.

Our CCSD calculations show convergence with respect to the single-particle basis size. For example, ^{5}He changes by only 300 keV (to -24.87 MeV) when we add *g*-orbitals. An extrapolation of the ^{5}He result to an infinite space using $E_N = \alpha \exp(-N/Nt) + E_\infty$, where N represents the space size, and α and Nt are fit parameters, yields $E_\infty = -24.89 \pm 0.01$ MeV. A similar fit for the ^{8}He data yields $E_\infty = -26.90 \pm 0.03$ MeV which is about 700 keV below the *s–g* calculations. Thus, the largest calculations we are performing appear to have good convergence with the number of basis states, and one is able to perform a simple exponential fit to obtain full space results with estimates on the extrapolation error. We note that the actual masses have a familiar pattern (based on $AV18$ results [30]) of underbinding as one increases the neutron number. As was found in GFMC calculations, this underbinding should mainly be overcome by the inclusion of three-body forces. We also compute the ground state expectation value of J^2. In the case of exact or variationally determined wave functions, the expectation value of an operator O can be evaluated via the Hellmann-Feynman theorem, $\frac{dE}{d\lambda}\big|_{\lambda=0} = \langle\psi(0)|O|\psi(0)\rangle$ by adding the small perturbation λO to the Hamiltonian. Though coupled-cluster theory is not a variational theory, the Hellmann-Feynman theorem is *effectively* fulfilled provided the ground state is determined with sufficient accuracy [32]. We find that the spins of all nuclei are well reproduced (to about one part in 1000) compared with experimental values, except for ^{6}He where the CCSD result is $J = 0.6$. It seems that a full CCSDT calculation would be needed to improve this expectation value.

	^{3}He		^{4}He		^{5}He		^{6}He		^{7}He		^{8}He		^{9}He		^{10}He	
lj	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]	Re[E]	Im[E]
$s-p$	-4.94	0.00	-24.97	0.00	-20.08	-0.54	-19.03	-0.18	-17.02	-0.24	-16.97	-0.00	-15.28	-0.40	-13.82	-0.12
$s-d$	-6.42	0.00	-26.58	0.00	-23.56	-0.22	-23.26	-0.09	-22.19	-0.12	-22.91	-0.00	-21.34	-0.15	-20.60	-0.02
$s-f$	-6.81	0.00	-27.27	0.00	-24.56	-0.17	-24.69	-0.07	-24.13	-0.11	-25.28	-0.00	-23.96	-0.06	-23.72	-0.00
$s-g$	-6.91	0.00	-27.35	0.00	-24.87	-0.16	-25.16	-0.06	-24.83	-0.09	-26.26	-0.00	-25.09	-0.03	-24.77	-0.00
Expt.	-7.72	0.00	-28.30	0.00	-27.41	-0.33(2)	-29.27	0.00	-28.83	-0.08(2)	-31.41	0.00	-30.14	-0.05(3)	-30.34	-0.09(6)

TABLE II: CCSD calculation of the $^{3-10}$He ground states with the low-momentum N^{3}LO nucleon-nucleon interaction for increasing number partial waves. The energies E are given in MeV for both real and imaginary parts. Experimental data are from Ref. [31].

In summary, we applied coupled-cluster theory for the *ab-initio* description of loosely bound and unbound nuclei. This is the first microscopic calculation that computes lifetimes of unstable nuclei from realistic nucleon-nucleon interactions. Using a renormalized interaction of the low-momentum type, basic properties of the helium chain are reproduced, i.e. ^{5,7}He unbound, ^{8}He bound and ^{6}He nearly bound at the CCSD level. The decay widths of unbound nuclei are in semiquantitative agreement with experimental data. For small model spaces, we could verify that the employed CCSD approximation agrees well with results from exact diagonalizations, and that CCSD(T) corrections improve our open-shell results. However, our CCSD(T) results for ^{6}He indicates that triples corrections cannot be treated perturbatively in the case of systems with a truly open-shell character. Different schemes for including triples corrections in these systems will be investigated in the future.

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